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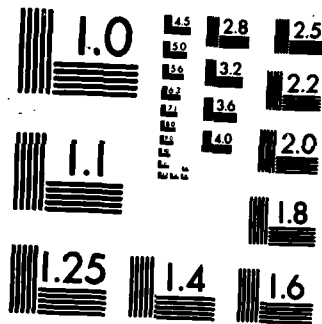
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Energy Disposal in Ion-Molecule Reactions:
Experiment and Theory

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Grant No: AFOSR-82-0035

Final Scientific Report

15 Nov 1981 to 14 May 1986

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FIELD	GROUP	SUB. GR.													
19. ABSTRACT (Continue on reverse if necessary and identify by block number) Work was completed in three areas: A. Kinetic Energy of Products of Simple Ion-Molecule Reactions; B. Internal Energy Dependence of Simple Bimolecular Ion-Molecule Reactions; C. Photodissociation Dynamics of Simple Ion-Neutral Clusters.															
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I. ABSTRACT

During the tenure of this grant work was accomplished in the 3 areas listed in the OBJECTIVES Section below. Summaries of this work have been given in the various Interim Reports and details are given in the attached complete set of reprints. In all 26 papers have been published and partial work completed on several additional projects. The work has been discussed at a large number of scientific meetings in both contributed and invited papers.

II. OBJECTIVES

A. Determination of Energy Disposal in Simple Unimolecular and Bimolecular Reactions.

B. Determination of the Effects of Internal Energy on the Rates and Branching Ratios of Bimolecular Reactions.

C. Determination of the Dynamics and energy Disposal in the Photodissociation of Simple Cluster Ions.

III. PROGRESS

Summaries of the work done are given in the various Interim Reports on file as well as the proposal submitted in Spring, 1985 (and subsequently funded as Grant AFOSR-86-0059). Consequently, a redundant summary of the work will not be given here. In the final few months of the grant work continued on a number of projects and preliminary results were obtained. Systems studied included photodissociation of the clusters $(\text{SO}_2)_2^-$ and KrSO_2^+ . The work has subsequently been completed and papers have been written and accepted for publication.

^{Superscript 2 P}
(4) Kinetic energy measurements on the products of reactions of $\text{C}_2^+ \text{P}$ with O_2 and NO were also initiated during the last months of AFOSR-82-0035. This work is essentially complete now and papers will be written shortly.

IV. PAPERS PUBLISHED OR IN PRESS

CUMULATIVE LIST

1981/82

1. Energy Disposal in Charge Transfer Reactions Producing NH_3^+ : Dependence of the $\text{NH}_3^+ + \text{H}_2\text{O}$ Reaction on NH_3^+ Internal Energy, P.R. Kemper, M.T. Bowers, D.C. Parent, G. Mauclaire, D. Deraï and R. Marx, J. Chem. Phys., **79**, 160 (1983).
2. Metastable Reactions in Small Cluster Ions, $(\text{CO}_2)_n^+$, $(\text{NH}_3)_2\text{H}^+$ and $(\text{H}_2\text{O})_2\text{H}^+$, A.J. Illies, M.F. Jarrold and M.T. Bowers, Int. J. Mass Spectrom. Ion Phys., **47**, 93 (1983).
3. Kinetics of Ion-Molecule Collision Complexes in the Gas Phase: Experiment and Theory, M.T. Bowers, M.F. Jarrold, W. Wagner-Redeker, P.R. Kemper and L.M. Bass, Faraday Discussion No. 75, 75/3 (1983).

4. Photodissociation of Vibrationally Excited CF_3I^+ . By a Single Infrared Photon, M.F. Jarrold, A.J. Illies, N.J. Kirchner, W. Wagner-Redeker, M.T. Bowers, M.L. Mandich and J.L. Beauchamp, J. Phys. Chem., **87**, 2213 (1983).

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5. Experimental and Theoretical Investigations of the Unimolecular Dissociation of Nascent Ion-Molecule Clusters: $\text{H}_2\text{O}\cdot\text{H}_3\text{O}^+$, $\text{NH}_3\cdot\text{NH}_4^+$ and $\text{CO}_2\cdot\text{CO}^+$, A.J. Illies, M.F. Jarrold, L.M. Bass and M.T. Bowers, J. Am. Chem. Soc., **105**, 5775 (1983).
6. On the Structure and Photodestruction of Cluster Ions in the Gas Phase: $(\text{N}_2)(\text{O}^+)$ and $(\text{NO})_2^+$, M.T. Bowers, A.J. Illies and M.F. Jarrold, Chem. Phys. Lett., **102**, 335 (1983).
7. Investigation of the Dynamics and Energy Disposal in the Photodissociation of Small Cluster Using a High Energy Ion Beam Crossed with a Laser Beam: Photodissociation of $(\text{NO})_2^+$ in the 488-660 nm Range, M.F. Jarrold, A.J. Illies and M.T. Bowers, J. Chem. Phys., **79**, 6086 (1983).
8. The Reaction of NH_3^+ with H_2S : Dependence on the Translational and Internal Energy of NH_3^+ , W. Wagner-Redeker, P.R. Kemper, M.T. Bowers and K.R. Jennings, J. Chem. Phys., **80**, 3606 (1984).
9. Energy Disposal in the Thermal and Near Thermal Energy Charge Exchange Reactions $\text{N}^+(\text{P}) + \text{CO}(\text{X}'\Sigma) \rightarrow \text{N}(\text{S}) + \text{CO}^+(\text{X}'\Sigma)$ and $\text{C}(\text{P}) + \text{NO}(\text{X}'\Sigma)$, A. O'Keefe, D. Parent, G. Mauclaire and M.T. Bowers, J. Chem. Phys., **80**, 4901 (1984).
10. The Dynamics of Photodissociation of Cluster Ions II: Photodissociation of the $(\text{NO})_3^+$ Cluster in the Visible Wavelength Range, M.F. Jarrold, A.J. Illies and M.T. Bowers, J. Chem. Phys., **81**, 222 (1984).
11. Energy Disposal in Photodissociation from Magic Angle Measurements with a Crossed High-energy Ion Beam and Laser Beam: Photodissociation Dynamics of the $(\text{N}_2)_2^+$ Cluster in the 458-514 nm Range, M.F. Jarrold, A.J. Illies and M.T. Bowers, J. Chem. Phys., **81**, 214 (1984).

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12. Electronic Predissociation of CrCO^+ and $\text{Cr}(\text{CO})_2^+$, M.F. Jarrold, L. Misev and M.T. Bowers, J. Phys. Chem., **88**, 3928 (1984).
13. Charge Transfer Half Collisions: Photodissociation of the $\text{Kr}\cdot\text{O}_2^+$ Cluster Ion with Resolution of the O_2 Product Vibrational States, M.F. Jarrold, L. Misev and M.T. Bowers, J. Chem. Phys., **81**, 4369 (1984).

14. Photodissociation of Gas Phase $(\text{CO})_2^+$ in the Visible Wavelength Range: Observation of Two Photodissociation Processes, A.J. Illies, M.F. Jarrold, W. Wagner-Redeker and M.T. Bowers, J. Phys. Chem., **88**, 5204 (1984).
15. Effect of Reactant Ion Internal and Translational Energy on the Rate Constants of Charge Exchange Reactions: $\text{CO}_2^+ + \text{O}_2 \rightarrow \text{O}_2^+ + \text{CO}_2$ and $\text{O}_2^+ + \text{O}_2 \rightarrow \text{O}_2 + \text{O}_2^+$, R. Derai, P.R. Kemper and M.T. Bowers, J. Chem. Phys., **82**, 4517 (1985).
16. Laser-Ion Beam Photodissociation Studies of C_6H_6^+ Radical Cations: The 2, 4-Hexadiyne System, R.K. Kravitt, D.H. Russell, M.F. Jarrold and M.T. Bowers, J. Am. Chem. Soc. **107**, 2346 (1985).
17. Fragmentation Dynamics and Energy Disposal in Photodissociation of $(\text{N}_2\text{O})_2^+$ in the 458-660 nm Wavelength Range, L. Misev, A.J. Illies, M.F. Jarrold and M.T. Bowers, Chem. Phys., **95**, 469 (1985).
18. Comparison of Energy Partitioning in Ar^+ and N_2^+ Charge Transfer Reactions, D.C. Parent, R. Derai, G. Mauclaire, M. Heninger, R. Marx, M.E. Rincon, A. O'Keefe and M.T. Bowers, Chem. Phys. Lett., **117**, 127 (1985).

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19. Product Energy Disposal in the Reaction of $\text{N}^+(^3\text{P}) + \text{O}_2(^1\Sigma)$, A. O'Keefe, G. Mauclaire D. Parent and M.T. Bowers, J. Chem. Phys., **84**, 215 (1986).

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20. Photodissociation of $\text{SO}_2 \cdot \text{SO}_2^+$ in the Visible Region of the Spectrum: Product Relative Kinetic Energy Distributions and Product Angular Distributions, M.F. Jarrold, A.J. Illies and M.T. Bowers, J. Chem. Phys., **82**, 1832 (1985).
21. Photoinduced Intramolecular Charge Transfer: Photodissociation of $\text{CO}_2^+ \cdot \text{Ar}$ Cluster Ions, A.J. Illies, M.F. Jarrold, W. Wagner-Redeker and M.T. Bowers, J. Am. Chem. Soc., **107**, 2842 (1985).
22. Photodissociation of Weakly Bound Ion-Molecule Clusters: The $\text{Kr} \cdot \text{CO}_2^+$ Cluster, M.F. Jarrold, A.J. Illies, W. Wagner-Redeker and M.T. Bowers, J. Chem. Phys., **89**, 3269 (1985).
23. Photodissociation of the Dimanganese ion Mn_2^+ : A Simple Route to the Dissociation Energies of Metal²Dimer Ions, M.F. Jarrold, A.J. Illies and M.T. Bowers, J. Am. Chem. Soc., **107**, 7339 (1985).
24. Reactions of Internally Excited, Energy Selected Ions, M.T.

Bowers, Adv. Mass Spectrometry, 10, 533 (1986).

25. Internal Energy Effects in Ion-Molecule Reactions: $\text{NH}_3^+ + \text{D}_2$, P.R. Kemper and M.T. Bowers, J. Phys. Chem., 90, 477 (1986).
26. A Laser-Ion Beam Study of the Photodissociation Dynamics of the $(\text{CO}_2)_3^+$ Cluster, H.-S. Kim, M.F. Jarrold and M.T. Bowers, J. Chem. Phys., 84, 4882.

*Not included in the list are the four papers mentioned in the Progress Section as these have not yet appeared in press.

V. PERSONNEL ASSOCIATED WITH THE PROJECT

Senior Research Personnel

Dr. Martin Jarrold	Dr. Winifred Wagner-Redeker
Dr. Andreas Illies	Dr. Lubomir Misev
Dr. Tony O'Keefe	Dr. Renee Deraï
Dr. Paul Kemper	Dr. Chau-Hong Kuo

Junior Research Personnel

Ms. Denise Parent	Ms. Marina Rincon
Mr. John Pearson	Ms. Hyun-Sook Kim

VI. PAPERS PRESENTED AT MEETINGS:

The various meetings at which both contributed and invited papers have been given on AFOSR sponsored research have been listed in previous interim reports. Here we list only a cumulative summary:

- A. Contributed papers given - 25
- B. Invited Symposium Lectures - 12
- C. University Seminars - 15



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